Detailed Simulations of Laboratory-Scale Premixed Turbulent Combustion

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SciDAC: Scientific Discovery through Advanced Computation

NOTE: Click images containing QT filmstrip icon to play a QuickTime movie

CCSE Research

Mission CCSE is an applied mathematics group that focuses on large-scale parallel simulation of complex fluid flows.

Expertise Mathematical analysis of multiphysics applications where advection is a key component, and design of appropriate high-resolution computational algorithms.

Applications

- Chemically reacting low- and high-speed flows
- Nuclear deflagrations
- Interface dynamics and turbulent mixing
- Explosion dynamics

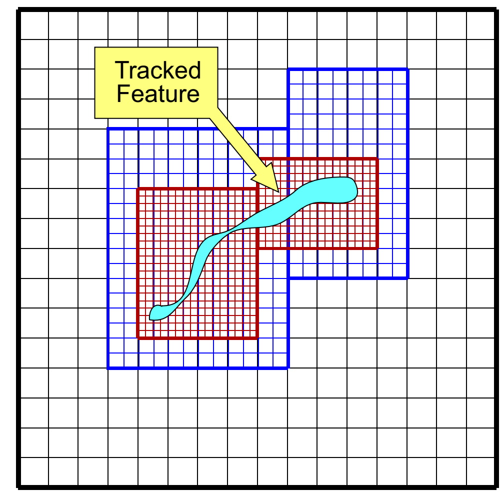
Framework Conservative finite-differences coupled to dynamically adapting meshes.

Block-Structured AMR

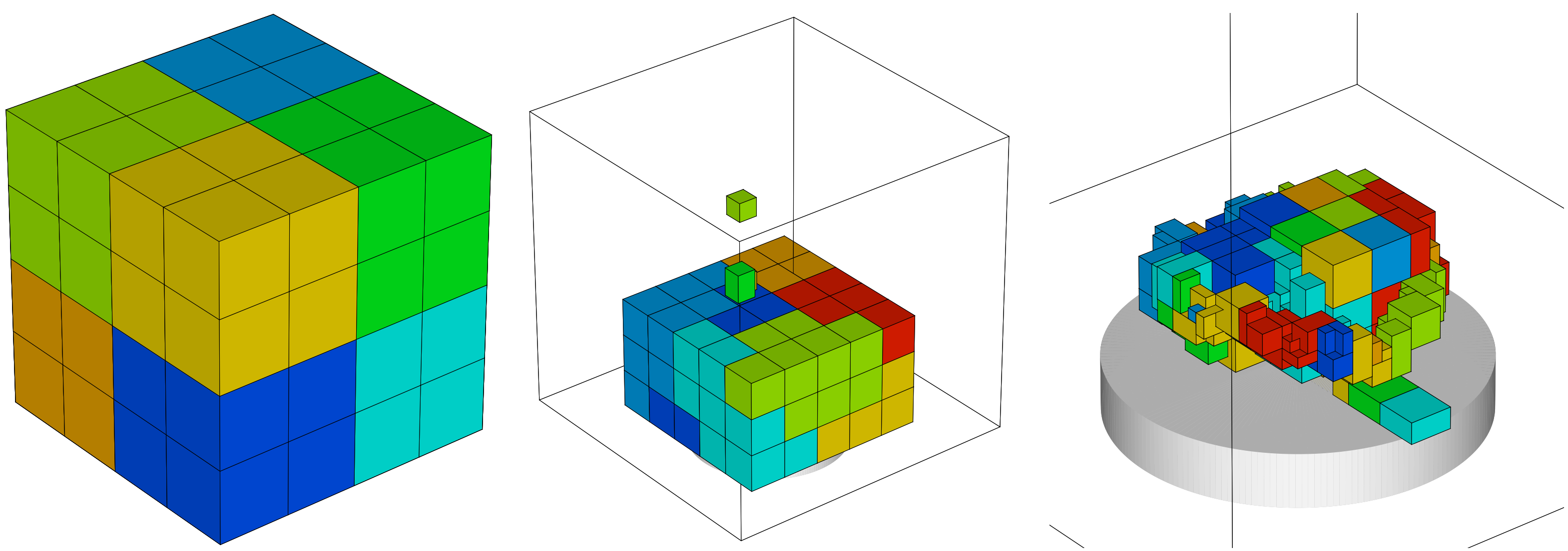
Each level is a union of rectangular patches

Each grid patch:

- Logically structured, rectangular
- Refined in space and time by evenly dividing coarse grid cells
- Dynamically created/destroyed to track time-dependent features
- In parallel, grids distributed based on work estimate



Block-structured hierarchical grids
(Berger and Colella, 1989)



Level 0 Level 1 Level 2

CCSE AMR Extensions

AMR - 14 years later...

- Parallel grid distribution, intra- and inter-level communication
- Variable property parabolic and elliptic AMR solvers
- Elliptically constrained flows, projection algorithms
- Time-split, sequential integration algorithms for complex applications
- AMAR (algorithm refinement) resolution-dependent models

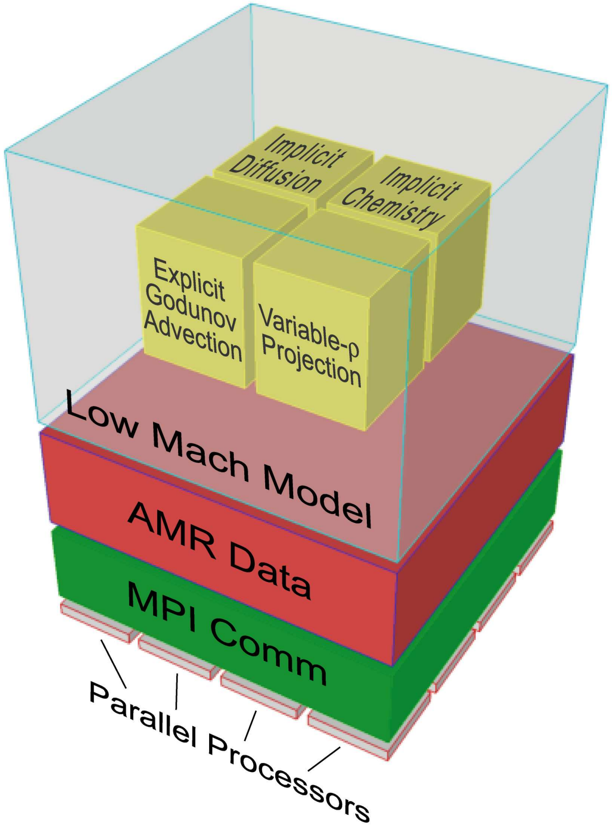
Example multiphysics applications:

1. Shock-induced mixing and combustion
2. Coupling Navier-Stokes to DSMC at the finest level
3. Variable-density shear layers, IAMR
4. Low Mach number laminar diffusion flames
5. Flame propagations in Type Ia supernovae
6. Nitric Oxide emissions in steady diffusion flames
7. Turbulent lean premixed methane combustion

Simulation Approach

For low detailed simulation of laboratory-scale burners:

- Low Mach number formulation
  - Eliminates acoustics, retains heating compressibility effects
  - Conserves species and enthalpy
- Adaptive mesh refinement
  - Localizes mesh where needed
  - Algorithm complexity
- Parallel architectures
  - Distributed memory
  - Dynamic load balancing
  - Heterogeneous work load



AMR Extensions - IAMR

Projection methods are a family of efficient algorithms for integrating systems satisfying the incompressibility constraint, $\nabla \cdot U = 0$.

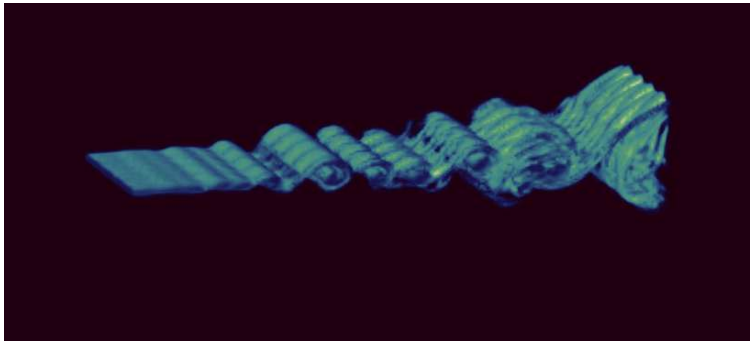
Projection methods are based on a 2-stage process:

1. Construct time-explicit update of U ignoring the $\nabla \cdot U = 0$ constraint
2. Extract the component of this update failing to satisfy the constraint

IAMR: Robust, conservative, adaptive-grid variable-ρ projection scheme

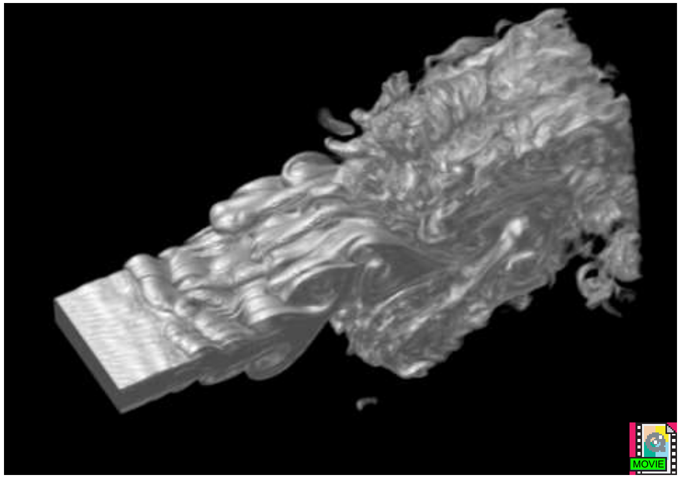
- Godunov advection
- Variable-coefficient Poisson solve
- Semi-implicit diffusion

Validation: Variable density shear layer



Brown and Roshko experiments (1974)

Example application of the IAMR algorithm



Evolution of an inert turbulent jet

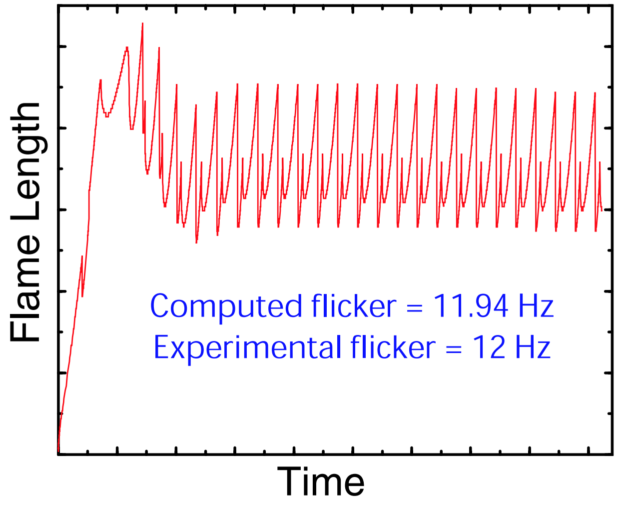
AMR Extensions - Laminar Flames

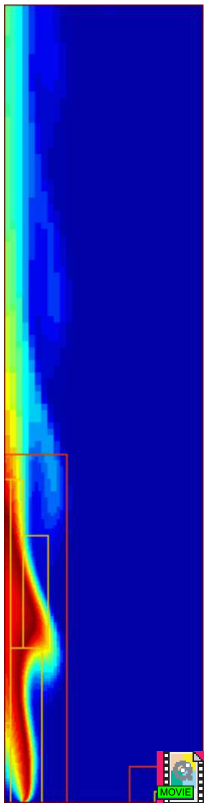
In many laboratory flames $U \ll C_s$. A *low Mach* model filters away acoustic waves, but leads to a elliptic constraint, $\nabla \cdot U = S$. Large time steps are traded for global coupling (linear solves) and algorithm complexity.

The IAMR adaptive projection algorithm extends naturally to low Mach number models for reacting flow.

Example: Flickering methane flame (buoyancy-driven K-H)

- Simple diffusion model
- Reduced chemistry
- Axisymmetric domain
- Grid refined T > 1800 K



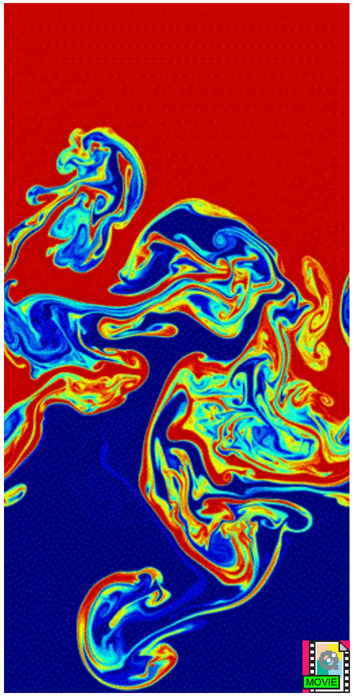


AMR Extensions - Type Ia Supernovae

Type Ia SNae: Detonation or constant-p deflagrations?

Can fluid dynamical instabilities increase effective burn rate?

A low Mach number simulation built by extending the laminar flame model.

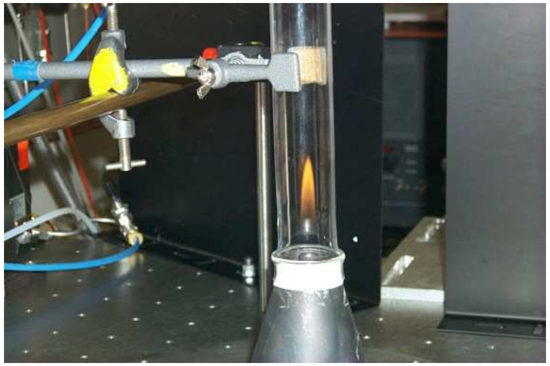


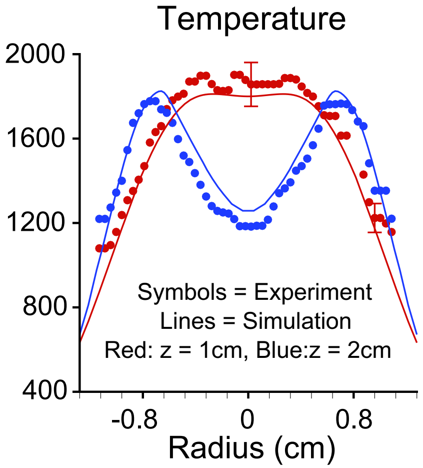
- Extensions: Degenerate EOS, nonlinear electron conduction, stiff nuclear chemistry, $^{12}\mathrm{C} \rightarrow {}^{24}\mathrm{Mg}$
- Here, $M \sim S_L/C_s \sim 10^{-3}$. Huge savings over DNS.

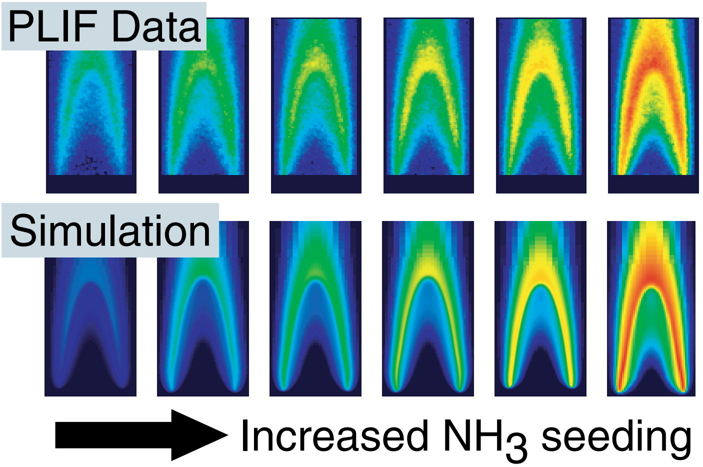
- Initial validation against FLASH (community standard)
- Long-time 2D integrations beyond FLASH capability
- Currently exploring first-ever 3D simulations

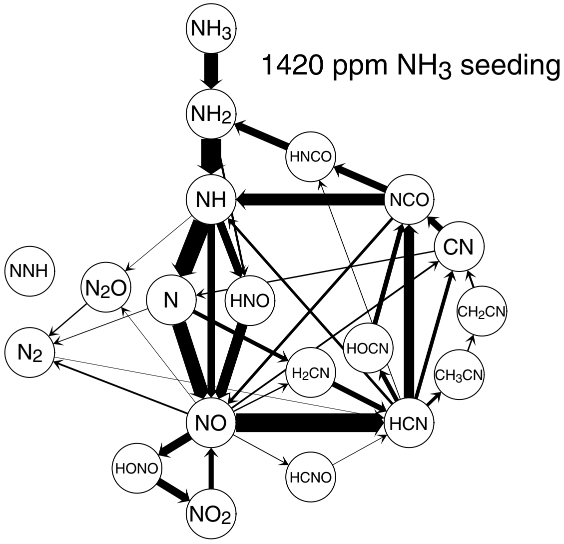
AMR Extensions - Detailed Flames

With the addition of detailed chemistry and transport, the fine-scaled structure of flame simulations can augment experimental diagnostics.







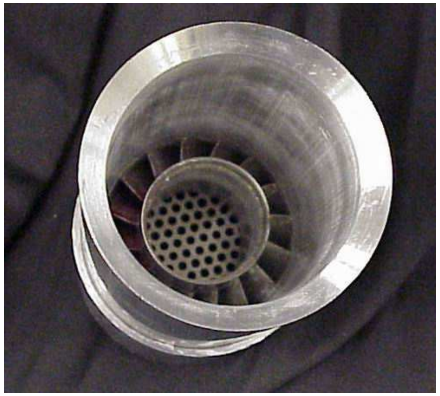


Lean Premixed Burners

LBNL Combustion Laboratories (R. Cheng)

Rod-stabilized V-flame

4-jet Low-swirl burner (LSB)

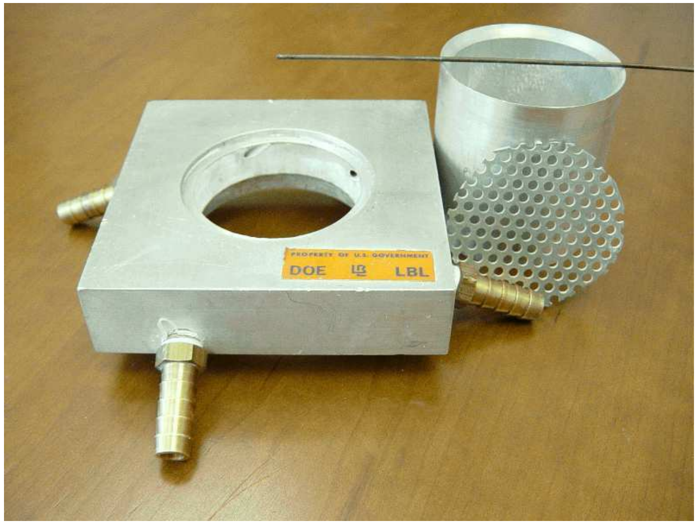


Industrial LSB nozzle

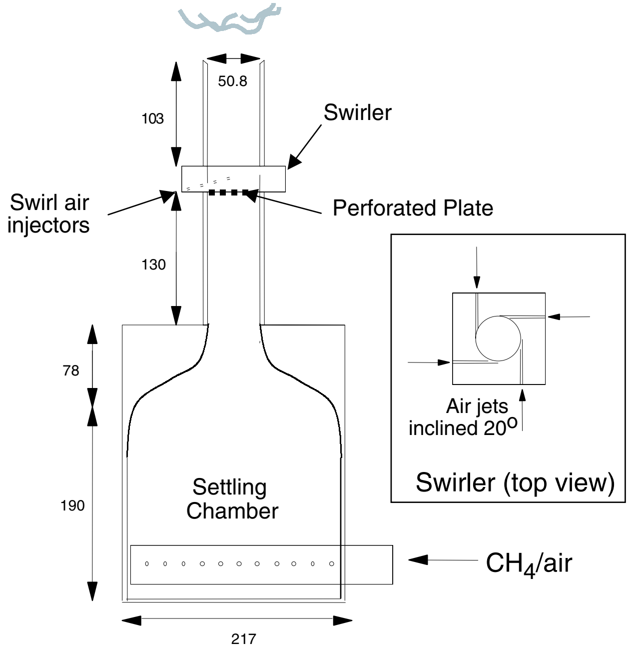
Support	Dept. of Energy, Office of Power Technologies
Mission	Develop low cost and robust methods for lean premixed combustion (LPC) to reduce NO_x in industrial burners
Technology	Aerodynamically stabilized LPC burners. Patented vane swirler demonstrated at industrial high-power conditions
Collaboration	Understand interaction of nozzle aerodynamics with flame propagation, turbulence and emission chemistry

Burner Configuration

- Same experimental device for LSB and V-flame
- Focus here on V-flames, no airflow through swirler jets
- Turbulence plate in nozzle has 3 mm holes on 4.8 mm centers



Burner assembly



Experiment schematic

Relevant Scales

Domain

- Fuel pipe $\sim$ 5 cm
- Flame length $\sim$ 20 cm
- Fueling rate $\sim$ 3 m/s
- Sound speed $\sim$ 350 m/s
- Exchange time $\sim$ 70 ms

Flame

- Thermal width $\sim$ 600 μm
- Reaction zone $\sim$ 150 μm
- C,H,O chemistry $\sim$ 10-1000 ns
- N chemistry $\sim$ .01 s
- Number species $\sim$ 20-80
- Number reactions $\sim$ 80-500

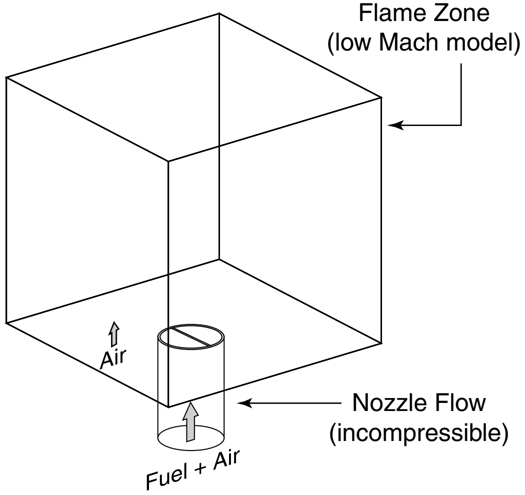
Turbulence

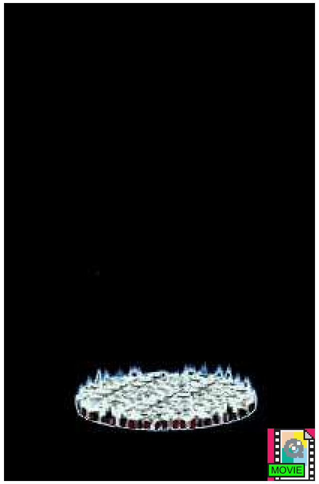
- Intensity $\sim$ 10-50 cm/s
- Viscous length $\sim$ 250 μm
- Coherent eddies $\sim$ 3-5 mm
- Eddy turnover $\sim$ 1 ms

Direct numerical simulation with reacting Navier-Stokes model

$\mathcal{O}(10^2)$species $\times$ $\mathcal{O}(10^{12})$cells $\times$ $\mathcal{O}(10^8)$steps

2-Part Simulation Strategy





1. Inert turbulent nozzle flow, IAMR

   Inflow Uniform inflow through perforated plate ("jet" array)

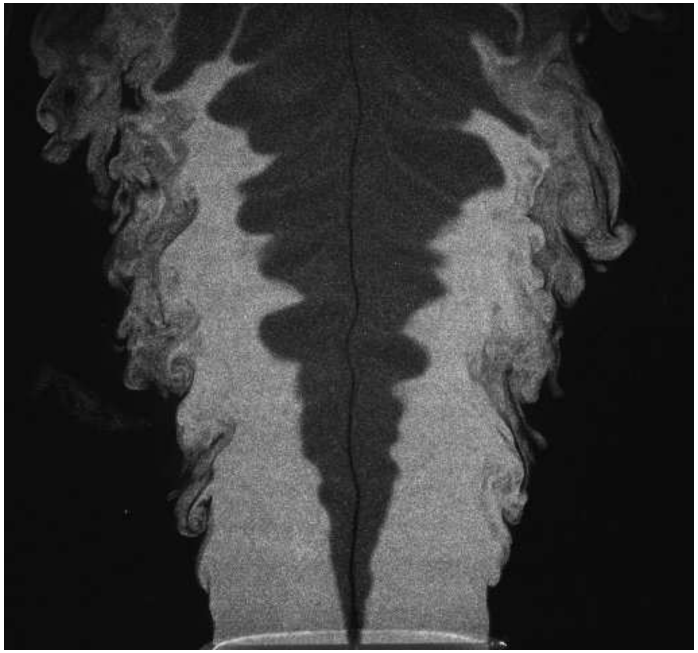
   Result After residence time $\sim L/U \sim$ 0.3s, breakup/mixing of inflow jets to nearly isotropic turbulence with thin boundary layers inside nozzle wall

2. Low Mach number reacting flow

   Inflow Data from step 1, but for small no-flow on rod surface

   Result Established flame at rod extends downstream and through outflow boundary

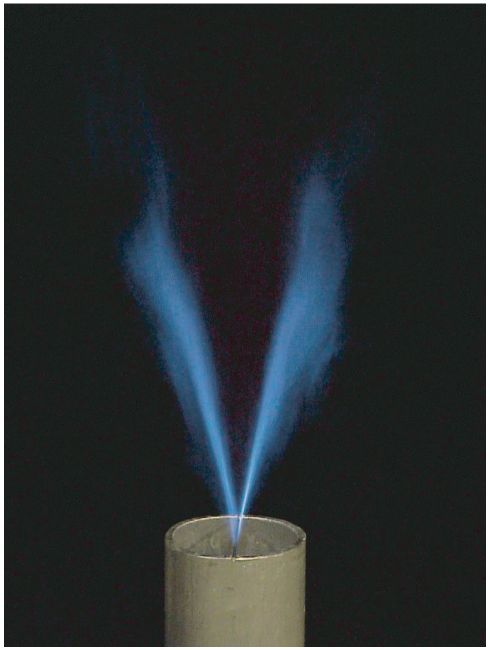
Results: Computation vs. Experiment

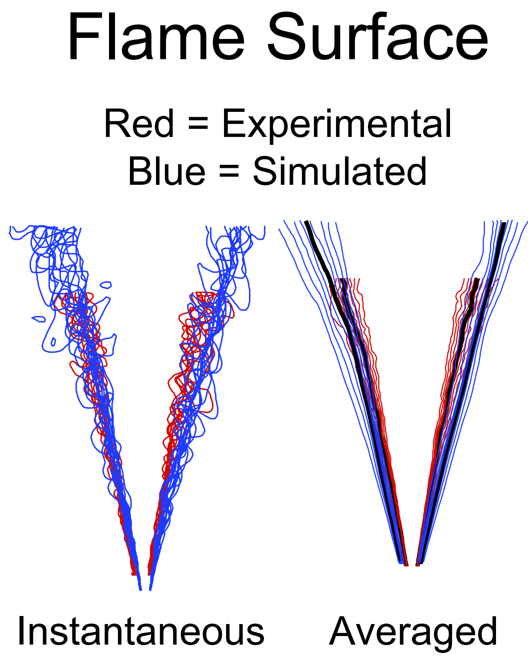


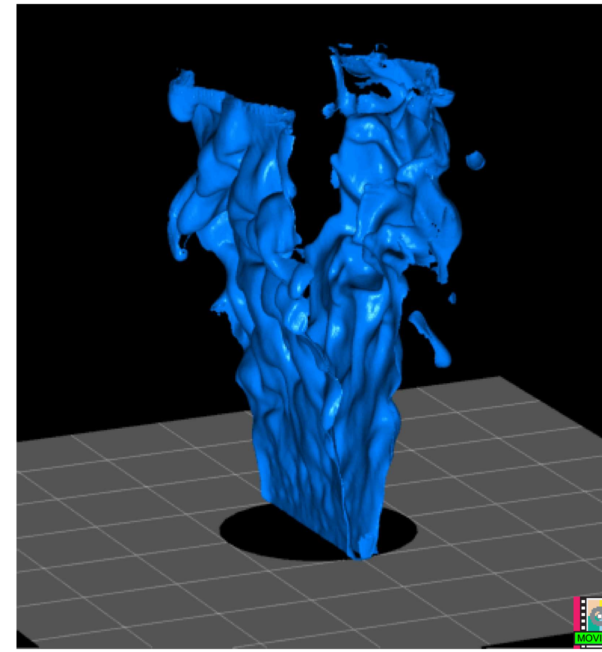
Experimental PIV image

CH_4 from simulation
(animation of density gradient field)

Instantaneous Flame Surface







Flame “location” depends on source of data:

Experiment: Find large ∇s, s = PIV particle density (indicates volumetric expansion)

Simulation: Find appropriate isosurface of $\|\nabla \rho\|$

V-Flame Simulation Stats

For the $\phi = 0.8$ run shown:

- 20 chemical species, 84 fundamental reactions
- 0.132 sec total simulated time, 1400 coarse-grid time steps
- Data generation: 3(4) AMR refinement levels, factor-of-2
  - Restart: 13 (60) GB/step, saved every 5th
  - Data analysis (38 quantities): 3.8 (16.8) GB/step, saved every 5th
  - Total (including refinement study): 6 TB
- AMR stats

Level	# grids	# cells	% Domain
0	27	885K	100
1	173	3.4M	48
2	870	9.2M	16
3	3700	46M	10

- Run on seaborg.nersc.gov, 256 CPUs, 2 steps/hr

Final Comments

Relationship to other work

- In the 2002 Proc. Combust. Symp, only 4 groups worldwide reported 3D detailed simulations of this sort
- All 3 other groups:
  1. Had access to vector-parallel computing hardware
  2. Used “traditional” (compressible DNS) methods
  3. Considered only hydrogen flames
- In 2003, CCSE is the only group capable of fully detailed simulations of laboratory-scale methane flames. Groups employing traditional simulation techniques are severely limited, even on vector-parallel supercomputers.

Future Work

- Continued validation work with experimentalists
- More detailed investigation of turbulent/flame interactions